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We have developed simulation tools for the optimization of the organic light-emitting device (OLED) high-resolution monochrome structures for medical imaging applications. We studied the effect of thin-film coatings and optical absorption in the organic materials on the emitted OLED spectra.
We investigated advanced measurement methods for the characterization of display prototypes that will be fabricated in the University of Michigan laboratories.
Using measured optical properties of the materials involved in a typical OLED structure, we computed the color shift from the photo-luminescent spectrum. In a submitted manuscript, we reported on the Monte Carlo method for modeling light transport phenomena in multi-layer organic polymer light-emitting devices on plastic substrates.
We find that for all polymers considered, the emission is shifted toward the longer wavelengths, and that the shift is maximum for emissions with peaks around 530 nm.
The photon extraction efficiency is higher (0.430) for polymers emitting in the longer wavelengths, while the absorbed fraction is higher (0.676) for spectra with maximum in the short wavelengths.

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3 Introduction

Commercially available display devices for use in digital mammography systems are known to have less image quality than the mammographic transilluminated film. Performance parameters that have been recognized as poor include low maximum luminance, reduced luminance range, veiling glare and ambient light reflections, insufficient resolution, and phosphor granularity noise, among others. The capacity of the display device to present all the information in a single image (as opposed to reduced views due to small display pixel array sizes), while maintaining the added bonuses of a digital technology (i.e., image processing) represents a significant improvement. Moreover, it is possible to achieve with an electronic display device better image quality than that observed with radiographic film.

CRTs constitute the only display device that is being used for clinical and diagnostic evaluation of digital medical images. Today, large-size five-Mpixel cathode-ray tubes (CRTs) are available from several manufacturers. Their low maximum luminance, insufficient dynamic range, high display reflectance and contrast-reducing veiling glare are significant sources of image quality degradation. Particularly for mammography, the resolution, luminance range and contrast modulation required has not been achieved by current systems. Active-matrix liquid crystal displays (AM-LCDs) have been developed with high resolution, large size, and good contrast performance have been achieved. However, such display quality is almost always quoted as a performance measurement given in the normal central direction with respect to the display. Severe degradation in the performance of the grey-scale and contrast is observed for off-axis viewing directions. These considerations suggest that the use of CRTs and AM-LCDs in mammography systems will go hand in hand with some suffering on image quality.

Organic polymer light-emitting displays (OLEDs) are all-solid-state flat panel devices that emit light through electron-hole recombination processes. Recently, OLEDs have received worldwide attention, because of their high luminous efficiency that can be achieved at room temperature with low driving voltages. A display device that delivers better image quality than the "gold standard" for mammography digital systems would allow a much more rapid and decisive deployment of fully digital solutions for the detection of breast cancer. The use of a display that could achieve a maximum luminance higher than 2,000 cd/m^2 while having a very low minimum luminance would allow the radiologists to implement image processing techniques that benefit from the extended luminance range. Such a display would allow for film-less practice without sacrificing diagnostic performance.

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The electronic display of mammographic images remains today an important technological barrier for the deployment of fully digital mammography systems. Extremely good spatial resolution in large image pixel array sizes are required to detect and characterize small lesions.

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In addition, good contrast resolution is needed to achieve high diagnostic performance when subtle details are present in low-luminance image regions [1,2]. The objective of this project is to develop a OLED that could replace mammographic film with improved display quality. Typically, an electronic display is associated with loss of image quality when compared to transilluminated film. This study will prove that an all-solid-state electronic display device can provide better image quality than film, while being thin, reliable and cost-effective. In the first year of this project, we have achieved the following objectives:

1. **Improved the available simulation methods for OLED modelling** by incorporate actual photon luminescent spectra characteristic of OLED materials used in the University of Michigan laboratory.

2. **Optimization of OLED optical performance**: We have developed advanced computational modelling tools to predict the achievable improvements and define new structures by studying the effect of surface and material properties on the optical performance of AM-OLEDs.

Optical design of the OLED has been the focus of recent interest [3–6]. In this work, we will use a Monte Carlo simulation code (DETECT-II) [7] to study the effect of light transport processes on the optical performance of the OLEDs. Monte Carlo methods track a large number of optical photons to describe the statistically averaged output. A unique advantage of this simulation method based on geometrical optics [8] is its ability to model absorption events, thin-film coatings and rough surfaces while keeping track of the photon polarization state [9]. Previously, we reported on the luminance spread functions of thin emissive displays showing that increased absorption in thin layers yield low veiling glare structures [10]. The current version of the simulation code models optically isotropic materials using a geometrical optics approach [9,10]. Light paths are assumed to apply to one single quanta (light photon). The reflection and transmission coefficients are therefore interpreted as probabilities.

Preliminary predictions suggest that about 80% of the light generated in the emissive layer is lost within the multi-layer stack and does not contribute to display luminance. Through this simulation, we will optimize the OLED multi-layer structure and thicknesses of different layers (including the substrate film). Moreover, the impact of optically thin films and rough surfaces has not yet been addressed in the published literature. We are now using DETECT-II to accurately simulate light transport in these multi-layer devices and to evaluate improvements in the stack design that can significantly improve the device efficiency and the viewing angle characteristics. Devices with an efficiency improved by a factor of 2-5 are achievable.

Recently, investigators have recognized that structured layers can significantly improve the efficiency and optical performance characteristics of OLED devices. For instance, Gu et al. have proposed to use a structured glass substrate to improve efficiency [4]. In this work, we propose to determine the exact optical properties of thin-film surfaces deposited with the same techniques that will be used for the OLED fabrication, using electron and atomic

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force microscopy. Special details will be collected for ITO thin films, substrates and metallic electrodes under different deposition conditions.

We submitted a manuscript to the Journal of Applied Physics with the results of this first phase of the research plan. In the paper, we reported on a Monte Carlo method for modelling light transport phenomena in multi-layer organic polymer light-emitting devices on plastic substrates. We applied the method to the analysis of the wavelength distribution of emitted spectra. A brief summary of the paper follows.

After the simple analysis of efficiency presented in Ref. 11, several groups have investigated the effect of light transport in multi-layer structures. [3–5, 12] The method we present in this paper, is based on a Monte Carlo (MC) approach. [7, 13] The MC method makes use of the generation of photons with random direction according to a distribution function describing the nature of the emission. In this analysis, the light source within the organic polymer layer is considered isotropic from a single point situated in the center of the device. To obtain an isotropic distribution of the directional cosines, we sample the three directional cosines that define the photon direction according to: $C_x = \sqrt{1 - \xi_1^2} sin2\pi\xi_2$, $C_y = \sqrt{1 - \xi_1^2} cos2\pi\xi_2$, $C_z = \xi_2$, where ξ_1 and ξ_2 are uniformly sampled in [0,1). The energy of the photon source is defined by a table corresponding to a specific spectral emission. The initial polarization vector is sampled uniformly in the 4π space, therefore assuming an unpolarized emission. The photon histories are then followed through a sequence of interactions that includes absorption, and Fresnel refraction. A unique advantage of this simulation method is its ability to model bulk absorption events, thin-film coatings and rough surfaces, while keeping track of the photon polarization state. Bulk absorption is determined by sampling the probability of a photon being absorbed after a path of length l by the exponential law $P(l) = 1 - exp^{-\mu_{ab}(\lambda)l}$, where $\mu_{ab}(\lambda)$ is the wavelength-dependent linear absorption coefficient. At the optical boundaries, an analysis is performed depending on the surface type and material properties, using Fresnel's equations and considering the polarization of the incoming photon. [8] When the film thickness is comparable to the photon wavelength, we use modified Fresnel coefficients to describe the interference effects of optically thin films. The reflection and transmission coefficients are then interpreted as probabilities. The simulation outcome is calculated by statistical average of the fate of all histories according to the desired quantity to be evaluated for each experiment. Possible reporting options include the angular and spectral distribution of the emitted photons, the point-spread function, the specular and diffuse reflection coefficients, and a summary of scattering events statistics.

From the emission at the luminescent center until the photons emerge, multiple scattering events take place within the multi-layer structure. For the purpose of our analysis, we define the device external quantum efficiency as: $\eta_E = \eta_{in} \eta_{pe}$, where η_{in} is the intrinsic efficiency related to carrier recombination and photo-luminescent fraction, and η_{pe} is the photon extraction efficiency. We introduce η_{pe} to represent the probability that a photon generated at the luminescent center emerges through the front surface of the device contributing to luminance. η_{pe} depends strongly on the device structure and on the material and surface properties, and is always less than unity due to absorption, wave-guiding, and edge-emissions.

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We can summarize the relevant physical processes that occur as $\eta_{pe} = 1 - \eta_{wa} - \eta_{ab} - \eta_{tr}$, where η_{wa} is the fraction of photons that are wave-guided within the structure and exit through the device edges, η_{ab} is the absorbed fraction, and η_{tr} is the fraction transmitted through the metallic electrode deposited in the side opposite to the direction of the desired emission. The top cathode electrode of all the structures modelled is an Aluminum coating deposited by vacuum evaporation. [14] We considered $\eta_{tr} = 0$ in all simulations presented in this paper.

We measured the index of refraction, absorption, photoluminescence (PL), and electroluminescence (EL) of three organic polymers (A, B, and C) with peak emission in a different region of the visible spectrum. We used the PL spectrum as the energy distribution at the source for the MC histories. The structure modelled in this paper is a hetero-structure OLED described in Ref. 14 with an aluminum cathode electrode and a transparent anode thin-film (160 nm, refractive index 1.8). The organic polymer film thickness used was 200 nm. The transparent substrate index of refraction was 1.5 and its thickness 900 μm. We present results on the simulated emission wavelength distribution (SL). For the three PL spectra considered, the measured EL spectrum is shifted toward the longer wavelengths. Our MC simulation results are consistent with this trend. By computing separately the simulated emission from a structure having absorption in the organic polymer film, and from another with no absorption but with a thin-film transparent layer between the organic material and the substrate, we have confirmed that the decrease in power in the shorter wavelength range is associated with the absorption in the organic material, while the increase in strength at longer wavelengths is caused by interference effects associated with the transparent conductive coating. Our simulation method can correctly predict the shift in maximum wavelength of each spectrum. However, specially in the longer wavelengths, a discrepancy exists between the EL and the MC calculated SL that cannot be explained in terms of optical transport phenomena.

The extraction efficiency η_{pe} is also affected by the wavelength distribution of the photon source. For the case with a transparent electrode having a thickness of 160 nm, and a refractive index of 1.80, η_{pe} is 0.314 for polymer A, 0.334 for polymer B, and 0.430 for polymer C. The absorbed fraction η_{ab} are 0.676, 0.655, and 0.553, and the wave-guided fraction η_{wa} is 0.001, 0.011, and 0.017, respectively for polymers A, B, and C. The low η_{wa} is caused by high absorption in the organic film. The waveguide modes are determined by the geometry of the stack of layers that define a total internal reflection angle (α_{TIR}) with respect to the device plane, beyond which all photons are emitted through the edges. Since our source of photons is isotropic, we expect lower η_{wa} for larger devices due to: (1) increased probability of reflection and scattering going into the solid angle defined by α_{TIR}, and (2) increased absorption in the organic polymer layer. The simulation result presented confirm this assumption. The results also confirm that since most of the wave-guiding occurs in the transparent substrate, the absorption in the organic polymer film has a minor effect on reducing edge-emission and increasing the extraction efficiency.

5 Key Research Accomplishments

In the first year of this project, we have achieved the following accomplishments:

1. **Improved the available simulation methods for OLED modelling** by incorporating actual photon luminescent spectra characteristic of OLED materials used in the University of Michigan laboratory.

2. **Optimization of OLED optical performance:** We studied the color shift of photoluminescent spectra generated for OLED materials used in our laboratories.

6 Reportable Outcomes

During the first stage of the research project, the simulation code was improved and ported to Windows-based computers and a variety of Unix machines (Sun UltraSparc 10, HP Vectra, etc). In the first year of this project, we generated one manuscript that was submitted for consideration to the Journal of Applied Physics (see Appendix).

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8 Appendices

Manuscript "MONTE CARLO ANALYSIS OF THE SPECTRAL PHOTON EMISSION AND EXTRACTION EFFICIENCY OF ORGANIC LIGHT-EMITTING DEVICES".